

Hyperfine interaction in a classical hydrogen atom and geometric quantization

C. DUVAL

Université d'Aix-Marseille II & Centre de Physique Théorique
CPT - CNRS Luminy - Case 907
F 13288 Marseille Cedex 9 France

J. ELHADAD

Université de Provence & Centre de Physique Théorique
CPT-CNRS Luminy - Case 907
F 13288 Marseille Cedex 9 France

G.M. TUYNMAN

Universiteit van Amsterdam
Mathematisch Instituut Roetersstraat 15
NL 1018 WB Amsterdam The Netherlands

Abstract. *We start with a Galilei-invariant symplectic model of two charged particles with spin and magnetic moment in interaction, which could serve as a model for the (classical) hydrogen atom. To this model we apply two different versions of geometric quantization and we obtain a hamiltonian operator which is (apart from some numerical constants) the well-known hamiltonian for the hydrogen atom, including spin-orbit coupling (fine-structure) and spin-spin interaction (hyperfine-structure).*

§ 1. THE CLASSICAL HYDROGEN ATOM

Let us recall that the movements of a classical (i.e. non-relativistic and not quantized) particle with spin under the influence of an exterior electromagnetic field are curves in the evolution space $E = \mathbb{R}^7 \times S^2$, curves who are the charac-

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teristics of a presymplectic 2-form σ (of rank 8) given by:

$$\begin{aligned}\sigma = & (m dv_j - e E_j dt) \wedge (dr^j - v^j dt) + \frac{1}{2} e \epsilon_{ijk} B^i dr^j \wedge dr^k \\ & - \frac{1}{2} s \epsilon_{ijk} u^i du^j \wedge du^k + d(\mu B_j u^j dt)\end{aligned}$$

with $(\mathbf{r}, \mathbf{v}, t) \in \mathbb{R}^7$, $\mathbf{u} \in S^2 \subset \mathbb{R}^3$ ($\|\mathbf{u}\| = 1$).

The quantities m , e , s and μ are constants which are interpreted as the mass, the electric charge, the spin and the magnetic moment associated to the spin vector of this particle. The electromagnetic field (\mathbf{E}, \mathbf{B}) is supposed to depend only on the space-time variables (\mathbf{r}, t) . The condition $d\sigma = 0$ leads us in particular to the homogeneous Maxwell equations, who guarantee the existence of the electromagnetic potentials (\mathbf{A}, V) such that $\mathbf{B} = \text{rot } \mathbf{A}$ and $\mathbf{E} = -\text{grad } V - \partial_t \mathbf{A}$.

With these definitions and the observation that $\frac{1}{2} \epsilon_{jkl} u^j du^k \wedge du^l = \sin \vartheta d\vartheta \wedge d\varphi = \text{surface}(S^2)$, the presymplectic form σ can be written as:

$$\sigma = d\{(m\mathbf{v} - e\mathbf{A}) \cdot d\mathbf{r} - H dt\} - s \cdot \text{surf}$$

where $H = \frac{1}{2} m \|\mathbf{v}\|^2 + eV - \mu \mathbf{B} \cdot \mathbf{u}$.

The equations of motion of this system are given by the characteristic foliation of σ , i.e. by $\ker(\sigma)$:

$$\begin{cases} \delta \mathbf{r} = \mathbf{v} \delta t \\ m \delta \mathbf{v} = [e(\mathbf{E} + \mathbf{v} \times \mathbf{B}) + \mu \text{grad}_{\mathbf{r}}(\mathbf{B} \cdot \mathbf{u})] \delta t \\ s \delta \mathbf{u} = \mu \mathbf{u} \times \mathbf{B} \delta t. \end{cases}$$

If we suppose that the electromagnetic field is created by a second particle of the same kind, then one derives finally (see [So2]) the following model: two particles in interaction with masses m_k , charges e_k , spins s_k and associated magnetic moments μ_k (where $k = 1, 2$) can be described by an evolution space E , which is an open set in $\mathbb{R}^{13} \times S^2 \times S^2$, and a presymplectic 2-form σ :

$$\sigma = d\omega - s_1 \cdot \text{surf}_1 - s_2 \cdot \text{surf}_2$$

with

$$\begin{aligned}(1.1) \quad \omega = & m_1 \mathbf{v}_1 \cdot d\mathbf{r}_1 + [\mathbf{u}^\# \times \mathbf{C}(\mathbf{r}_1 - \mathbf{r}_2)] \cdot d\mathbf{r}_1 \\ & + m_2 \mathbf{v}_2 \cdot d\mathbf{r}_2 + [\mathbf{u}^\# \times \mathbf{C}(\mathbf{r}_2 - \mathbf{r}_1)] \cdot d\mathbf{r}_2 - H dt\end{aligned}$$

$$H = \frac{1}{2} m_1 \|\mathbf{v}_1\|^2 + \frac{1}{2} m_2 \|\mathbf{v}_2\|^2 + e_1 e_2 V(\mathbf{r}_1 - \mathbf{r}_2) + \mu_1 \mu_2 \mathbf{u}_1 \cdot \mathbf{C}'(\mathbf{r}_1 - \mathbf{r}_2) \cdot \mathbf{u}_2$$

where we have introduced the following useful abbreviations:

$$(1.2) \quad \begin{cases} \mathbf{u}^\# = \lambda_1 \mathbf{u}_1 + \lambda_2 \mathbf{u}_2, & \lambda_1 = k \mu_1 e_2, \quad \lambda_2 = k \mu_2 e_1, \quad k = c^{-1} \\ V(\mathbf{q}) = \|\mathbf{q}\|^{-1}, & \mathbf{C}(\mathbf{q}) = -\mathbf{grad}_{\mathbf{q}} V(\mathbf{q}) = \mathbf{q} \cdot \|\mathbf{q}\|^{-3} \\ \mathbf{C}'(\mathbf{q}) = \mathbf{1} \cdot \|\mathbf{q}\|^{-3} - 3 \mathbf{q} \cdot \mathbf{q}^T \cdot \|\mathbf{q}\|^{-5}. \end{cases}$$

One easily verifies that σ is invariant under the action of the Galilei group:

$$\begin{cases} \mathbf{r}_k \rightarrow A \mathbf{r}_k + \mathbf{b}t + \mathbf{c} \\ \mathbf{v}_k \rightarrow A \mathbf{v}_k + \mathbf{b} \\ \mathbf{u}_k \rightarrow A \mathbf{u}_k \\ t \rightarrow t + \tau \\ A \in SO(3), \quad \mathbf{b}, \mathbf{c} \in \mathbb{R}^3, \quad \tau \in \mathbb{R} \end{cases}$$

hence the general theorem on barycentric decomposition can be applied (see [Sol1]), which results in the following obvious change of coordinates:

$$\begin{cases} \mathbf{R} = (m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2)/M \\ \mathbf{V} = (m_1 \mathbf{v}_1 + m_2 \mathbf{v}_2)/M \\ \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \\ \mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2 \\ M = m_1 + m_2, \quad m = m_1 m_2 / M. \end{cases}$$

In these coordinates the 1-form ω (1.1) takes the form:

$$(1.3) \quad \omega = (M \mathbf{V} \cdot d\mathbf{R} - H_b dt) + (m \mathbf{v} \cdot d\mathbf{r} + [\mathbf{u}^\# \times \mathbf{C}(\mathbf{r})] \cdot d\mathbf{r} - H_r dt)$$

$$H_b = \frac{1}{2} M \|\mathbf{V}\|^2$$

$$(1.4) \quad H_r = \frac{1}{2} m \|\mathbf{v}\|^2 + e_1 e_2 V(\mathbf{r}) + \mu_1 \mu_2 \mathbf{u}_1 \cdot \mathbf{C}'(\mathbf{r}) \cdot \mathbf{u}_2$$

This model was proposed by Souriau to describe the hydrogen atom in terms which are purely classical. If we forget the movement of the barycentre (which is rectilinear with constant velocity), we obtain a reduced evolution space

$E_r = \mathbb{R}^3 \setminus \{0\} \times \mathbb{R}^3 \times \mathbb{R} \times S^2 \times S^2$ containing the point $(\mathbf{r}, \mathbf{v}, t, \mathbf{u}_1, \mathbf{u}_2)$ with presymplectic 2-form σ_r :

$$(1.5) \quad \sigma_r = d\omega_r - s_1 \cdot \text{surf}_1 - s_2 \cdot \text{surf}_2$$

$$(1.6) \quad \omega_r = [m\mathbf{v} + \mathbf{u}^\# \times \mathbf{C}(\mathbf{r})] \cdot d\mathbf{r} - H_r dt.$$

This system has $SO(3) \times \mathbb{R}$ as a dynamical group and the associated momentum-mapping ([Sol]) gives us 4 conserved (Noether) quantities: the energy H_r and the total angular momentum $\mathbf{L}_{r,\text{tot}}$:

$$(1.7) \quad \mathbf{L}_{r,\text{tot}} = \mathbf{r} \times [m\mathbf{v} + \mathbf{u}^\# \times \mathbf{C}(\mathbf{r})] + s_1 \mathbf{u}_1 + s_2 \mathbf{u}_2.$$

Since we will be interested only in the reduced model, in the sequel we will drop the subscript r , so from now on we work with an evolution space $E \subset \mathbb{R}^7 \times S^2 \times S^2$, together with a presymplectic 2-form σ defined by (1.5). The formulas (1.6) and (1.7) strongly suggest the introduction of the coordinates $\mathbf{p} = m\mathbf{v} + \mathbf{u}^\# \times \mathbf{C}(\mathbf{r})$ instead of \mathbf{v} and indeed the gives:

$$(1.8) \quad \left\{ \begin{array}{l} \sigma = d\mathbf{p} \wedge d\mathbf{r} - s_1 \cdot \text{surf}_1 - s_2 \cdot \text{surf}_2 - dH \wedge dt \\ \mathbf{L}_{\text{tot}} = \mathbf{r} \times \mathbf{p} + s_1 \mathbf{u}_1 + s_2 \mathbf{u}_2 \\ H = \|\mathbf{p}\|^2/2m + e_1 e_2 V(\mathbf{r}) + \mathbf{u}^\# \cdot (\mathbf{C}(\mathbf{r}) \times \mathbf{p})/m \\ \quad + \mu_1 \mu_2 \mathbf{u}_1 \cdot \mathbf{C}'(\mathbf{r}) \cdot \mathbf{u}_2 + \|\mathbf{u}^\# \times \mathbf{C}(\mathbf{r})\|^2/2m. \end{array} \right.$$

In σ one should recognise the canonical part $d\mathbf{p} \wedge d\mathbf{r}$, in \mathbf{L} one recognises the usual angular momentum plus the two internal angular momenta usually called spin, and finally H should be compared to usual hamiltonian-operator of the hydrogen atom: kinetic energy, Coulomb potential, spin-orbit coupling, spin-interaction and the diamagnetic term.

The equations of motion are again given by $\ker(\sigma)$, i.e.:

$$(1.9) \quad \left\{ \begin{array}{l} \delta\mathbf{r}/\delta t = \mathbf{v} = (\mathbf{p} - \mathbf{u}^\# \times \mathbf{C}(\mathbf{r}))/m \\ s_1 \delta\mathbf{u}_1/\delta t = [\lambda_1 \mathbf{v} \times \mathbf{C}(\mathbf{r}) + \mu_1 \mu_2 \mathbf{C}'(\mathbf{r}) \cdot \mathbf{u}_2] \times \mathbf{u}_1 \\ s_2 \delta\mathbf{u}_2/\delta t = [\lambda_2 \mathbf{v} \times \mathbf{C}(\mathbf{r}) + \mu_1 \mu_2 \mathbf{C}'(\mathbf{r}) \cdot \mathbf{u}_1] \times \mathbf{u}_2 \\ \delta\mathbf{p}/\delta t = \mathbf{C}'(\mathbf{r}) \cdot [\mathbf{v} \times \mathbf{u}^\#] + e_1 e_2 \mathbf{C}(\mathbf{r}) - \mu_1 \mu_2 \mathbf{u}_1 \cdot \mathbf{C}''(\mathbf{r}) \cdot \mathbf{u}_2 \end{array} \right.$$

where $\mathbf{a} \cdot \mathbf{C}''(\mathbf{r}) \cdot \mathbf{b} = -3 \|\mathbf{r}\|^{-5} [(\mathbf{r} \cdot \mathbf{a}) \mathbf{b} + (\mathbf{r} \cdot \mathbf{b}) \mathbf{a} + (\mathbf{a} \cdot \mathbf{b}) \mathbf{r}] + 15 \|\mathbf{r}\|^{-7} (\mathbf{r} \cdot \mathbf{a})(\mathbf{r} \cdot \mathbf{b}) \mathbf{r}$.

Associated to this evolution space E is a phase space M , which is a leaf $t = \text{constant}$ of E . The pull-back of σ to M is a symplectic form, which we will denote also by σ , and the equations of motion are given by the flow of the hamiltonian vectorfield X_H associated to the hamiltonian H (which is defined on M

since H does not depend on t) by $\sigma(X_H, \cdot) + dH = 0$.

§2. PREQUANTIZATION

Prequantization is the intermediate step between a classical description of a system (by a symplectic manifold and a hamiltonian) and the corresponding quantum mechanical description derived by means of geometric quantization. It should be noted at this point that there exist two (nearly) equivalent viewpoints of geometric quantization: one by Souriau and one by Kostant (e.a.). In this and subsequent sections we will describe briefly the necessary ingredients of these two viewpoints, specialising to the model we want to study, i.e. the reduced hydrogen atom as described in §1. For a more detailed account of these two quantization procedures the reader is referred to [So1] and [Du] for Souriau's approach, and to [Bl], [Ko1] and [Ko2], or to [S&W], [Sn], [Wo], [Tu1], [Tu2] for the approach by Kostant and others.

§2a. PREQUANTIZATION ACCORDING TO SOURIAU

A prequantization of a symplectic manifold (M, σ) is a pair (Y, α) in which $\pi : Y \rightarrow M$ is a principal $U(1) = S^1 \subset \mathbb{C}$ bundle over M and α/\hbar a connection-form on Y with associated curvature form $\text{curv}(\alpha/\hbar) = (\pi^*\sigma)/\hbar$.

If $M = S^2$, $\sigma = -s \cdot \text{surf}(S^2)$ then M admits a prequantization only if $s = \frac{1}{2} n\hbar$, $n \in \mathbb{Z} \setminus \{0\}$. To describe such a prequantization we recall the Hopf fibration $\pi : S^3 \rightarrow S^2$ which can be defined as follows:

$$\mathbf{Z} \in S^3 \subset \mathbb{C}^2 \Leftrightarrow \mathbf{Z} = \begin{pmatrix} Z^1 \\ Z^2 \end{pmatrix}, \mathbf{Z}^\dagger = (Z^{1\dagger}, Z^{2\dagger}), \mathbf{Z}^\dagger \cdot \mathbf{Z} = 1 \quad (\dagger \text{ denotes complex-conjugation and transposition})$$

$$\Leftrightarrow 2\mathbf{Z} \cdot \mathbf{Z}^\dagger - \mathbf{1} \in GL(2, \mathbb{C}) \text{ is a hermitian involution with zero trace}$$

$$\Rightarrow \exists! \mathbf{u} \in S^2 \subset \mathbb{R}^3 : 2\mathbf{Z} \cdot \mathbf{Z}^\dagger - \mathbf{1} = \mathbf{u} \cdot \boldsymbol{\sigma}$$

$$\text{with } \boldsymbol{\sigma} = \text{Pauli-matrices} = (\sigma^1, \sigma^2, \sigma^3) = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right).$$

Now $\pi(\mathbf{Z}) = \mathbf{u}$ is a well defined projection which turns S^3 into a $U(1)$ bundle over S^2 , because π is invariant under the action of $U(1)$ on S^3 defined by scalar times vector:

$$\left. \begin{array}{l} \zeta \in U(1) \subset \mathbb{C}, |\zeta| = 1 \\ \mathbf{Z} \in \mathbb{C}^2, \mathbf{Z}^\dagger \cdot \mathbf{Z} = 1 \end{array} \right\} \Rightarrow 2\mathbf{Z} \cdot \mathbf{Z}^\dagger - 1 = 2(\mathbf{Z}\zeta) \cdot (\mathbf{Z}\zeta)^\dagger - 1 \Rightarrow \pi(\mathbf{Z}) = \pi(\mathbf{Z}\zeta)$$

and because this is the only freedom in \mathbf{Z} when $\pi(\mathbf{Z})$ is given.

The group $\mathbb{Z}/n\mathbb{Z}$ can be considered as a subgroup of $U(1)$ and $U(1) \bmod (\mathbb{Z}/n\mathbb{Z}) \cong U(1)$, so we can construct $U(1)$ bundles Y_n over S^2 by

$$Y_n = S^3/(\mathbb{Z}/n\mathbb{Z}).$$

The 1-form α_n on S^3 defined by $\alpha_n = i n \hbar \mathbf{Z}^\dagger \cdot d\mathbf{Z}$ descends to Y_n and (Y_n, α_n) defines a prequantization of $\left(S^2, -\frac{1}{2} n \hbar \cdot \text{surf}\right)$.

The case in which we are interested is the symplectic manifold $M = T^*Q \times S^2 \times S^2$ with configuration space $Q = \mathbb{R}^3 \setminus \{0\}$ and the symplectic form σ given by (1.5) or (1.8) (at $t = \text{constant}$). One can verify (see [Sol]: quantization by fusion) that a prequantization (Y, α) of this system is given by:

$$Y = T^*Q \times S^3 \times S^3 / \sim$$

where

$$(\mathbf{r}, \mathbf{v}, \mathbf{Z}_1, \mathbf{Z}_2) \sim (\mathbf{r}, \mathbf{v}, \mathbf{Z}_1 \zeta \exp(2\pi i k_1/n_1), \mathbf{Z}_2 \zeta^{-1} \exp(2\pi i k_2/n_2))$$

for

$$\zeta \in U(1), \quad k_i \in \mathbb{Z}, \quad s_i = \frac{1}{2} n_i \hbar, \quad (i = 1, 2)$$

and a 1-form α on Y which is the direct image of the 1-form β on $T^*Q \times S^3 \times S^3$:

$$\beta = [m\mathbf{v} + \mathbf{u}^\# \times \mathbf{C}(\mathbf{r})] \cdot d\mathbf{r} + i n_1 \hbar \mathbf{Z}_1^\dagger \cdot d\mathbf{Z}_1 + i n_2 \hbar \mathbf{Z}_2^\dagger \cdot d\mathbf{Z}_2.$$

It should be noted that any other prequantization (Y', α') of this system is equivalent to the given one since M is simply connected (which implies that $H^1(M, \mathbb{T}) = 0$ and this cohomology space indexes all inequivalent prequantizations).

The hamiltonian vectorfield X_H of H (see (1.4) or (1.8)) on M can be lifted to a vectorfield \hat{X}_H on Y in a unique way such that

$$\alpha(\hat{X}_H) = \pi^*H \quad \text{and} \quad \pi_*\hat{X}_H = X_H.$$

When we restrict ourselves to the case which is particularly interesting: $s_1 =$

$s_2 = \frac{1}{2} \hbar$ one finds for \hat{X}_H :

$$(2.1) \quad \left\{ \begin{array}{l} \delta \mathbf{r} = \mathbf{v} \\ \delta \mathbf{v} = m^{-1} \{ \mathbf{C}(\mathbf{r}) \times \delta \mathbf{u}^\# - \mathbf{u}^\# \times [\mathbf{C}'(\mathbf{r}) \cdot \mathbf{v}] - \mathbf{C}'(\mathbf{r}) \cdot [\mathbf{u}^\# \times \mathbf{v}] \\ \quad + e_1 e_2 \mathbf{C}(\mathbf{r}) - \mu_1 \mu_2 \mathbf{u}_1 \cdot \mathbf{C}''(\mathbf{r}) \cdot \mathbf{u}_2 \} \\ \delta \mathbf{Z}_1 = i/\hbar \{ v_1 \mathbf{Z}_1 + ([\lambda_1 \mathbf{C}(\mathbf{r}) \times \mathbf{v} - \mu_1 \mu_2 \mathbf{C}'(\mathbf{r}) \mathbf{u}_2] \cdot \sigma) \mathbf{Z}_1 \} \\ \delta \mathbf{Z}_2 = i/\hbar \{ v_2 \mathbf{Z}_2 + ([\lambda_2 \mathbf{C}(\mathbf{r}) \times \mathbf{v} - \mu_1 \mu_2 \mathbf{C}'(\mathbf{r}) \mathbf{u}_1] \cdot \sigma) \mathbf{Z}_2 \} \\ v \equiv v_1 + v_2 = 1/2 m \|\mathbf{v}\|^2 - e_1 e_2 V(\mathbf{r}) + \mu_1 \mu_2 \mathbf{u}_1 \mathbf{C}'(\mathbf{r}) \mathbf{u}_2 \\ \quad = H - 2e_1 e_2 V(\mathbf{r}) \quad (\text{c.f. (1.4)}) \end{array} \right.$$

where $\delta \mathbf{u}^\#$ is given by (1.2) and (1.9) with $\delta t = 1$.

In this formula v_1 and v_2 are two real Lagrange multipliers; their remaining arbitrariness ($v_1 - v_2$) disappears when passing to the quotient Y .

§2b. PREQUANTIZATION ACCORDING TO KOSTANT

In this formalism a prequantization of a symplectic manifold (M, σ) is a complex line-bundle L over M with connection ∇ and compatible fibre-inner product such that curvature $(\nabla) = \sigma/\hbar$. The connection between this formalism and Souriau's is that $\pi : L \rightarrow M$ is the vector bundle associated to the principal $U(1)$ bundle Y by means of the standard action of $U(1)$ on \mathbb{C} ; the connection ∇ on L is then derived from the connection form α/\hbar on Y .

If $M = S^2$, $\sigma = -s \cdot \text{surf}$ the bundle L is trivialised by means of two local charts $U_\pm = \mathbb{R}^2 = \mathbb{C}$ on M with transition function $z_- = 1/z_+$ (i.e. U_\pm are the two natural charts on $S^2 = \mathbb{P}^1(\mathbb{C})$, where z_+ is the projection from the north pole of S^2 and z_- the projection from the south pole followed by an inversion; the local coordinate z_+ is related to the coordinates (Z^1, Z^2) defined in the beginning of §2a by $z_+^\dagger = Z^1/Z^2$). Local charts of L are now given by $U_\pm \times \mathbb{C}$ with transition function:

$$U_+ \times \mathbb{C} \ni (m, w) \rightarrow (m, g_{-+}(m)w) \in U_- \times \mathbb{C},$$

$$g_{-+}(m) = (z_+ / |z_+|)^{-2s/\hbar} = (z_- / |z_-|)^{2s/\hbar} = \exp(-2is\varphi_+/\hbar) = \exp(2is\varphi_-/\hbar).$$

From this formula one can see the origin of the quantization condition $2s/\hbar \in \mathbb{Z}$: this is a necessary condition to guarantee that this transition function is well defined on S^2 .

A section λ of L is represented by two complex functions λ_\pm on U_\pm and the connection ∇ acting on λ is defined by means of local symplectic potentials ϑ_\pm (i.e. $d\vartheta_\pm = \sigma = -s \cdot \text{surf}$): for a (local) vectorfield ξ on M :

$$(\nabla_{\xi} \lambda)_{\pm} = \xi \lambda_{\pm} - i/\hbar \vartheta_{\pm}(\xi) \lambda_{\pm}$$

$$\vartheta_{\pm} = is (z_{\pm} z_{\pm}^{\dagger} + 1)^{-1} (z_{\pm} dz_{\pm}^{\dagger} - z_{\pm}^{\dagger} dz_{\pm}) \quad \sigma = 2is (z_{\pm} z_{\pm}^{\dagger} + 1)^{-2} dz_{\pm} \wedge dz_{\pm}^{\dagger}.$$

In our case $M = T^*Q \times S^2 \times S^2$, $Q = \mathbb{R}^3 \setminus \{0\}$, and σ given by (1.5) or (1.8) (at $t = \text{const}$), and a trivialisation of L is given over four charts $U_{\pm\pm} = T^*Q \times U_{\pm} \times U_{\pm}$ with transition functions $g_{(\pm\pm)(\pm\pm)}$ given by e.g.:

$$g_{(-+)(-+)}(m) = \exp(-2is_2\varphi_{2+}/\hbar), \quad g_{(+ -)(+ -)}(m) = \exp(2i(s_1\varphi_{1+} + s_2\varphi_{2-})/\hbar).$$

The connection ∇ is given on local sections $\lambda_{\pm\pm}$ by the formula:

$$\begin{aligned} (\nabla_{\xi} \lambda)_{\pm\pm} &= \xi \lambda_{\pm\pm} - i/\hbar \vartheta_{\pm\pm}(\xi) \lambda_{\pm\pm} \\ \vartheta_{\pm\pm} &= \mathbf{p} \cdot d\mathbf{r} + is_1(z_{1\pm} z_{1\pm}^{\dagger} + 1)^{-1} (z_{1\pm} dz_{1\pm}^{\dagger} - z_{1\pm}^{\dagger} dz_{1\pm}) \\ &\quad + is_2(z_{2\pm} z_{2\pm}^{\dagger} + 1)^{-1} (z_{2\pm} dz_{2\pm}^{\dagger} - z_{2\pm}^{\dagger} dz_{2\pm}). \end{aligned}$$

Other choices of local symplectic potentials ϑ correspond to different trivialisations of the same bundle L (since there is only one such bundle up to equivalence).

§3. POLARIZATIONS

One can associate in a canonical way a Hilbert-space H_c to a prequantization (in the formalism of either Souriau or Kostant) with the nice property that to each observable f , $f: M \rightarrow \mathbb{R}$, corresponds an operator Q_f on H_c satisfying the commutation relation

$$Q_{[f,g]} = i/\hbar [Q_f, Q_g]$$

(with on the left-hand side the Poisson-bracket of f and g and on the right-hand side the commutator of operators), together with $Q_1 = 1$. However H_c cannot serve as the Hilbert-space representing the quantummechanical description of the system since it consists essentially of functions on M and not of functions of the position coordinates only (or the momentum coordinates only).

The key-idea is to replace H_c by a Hilbert-space H consisting of (roughly speaking) functions which depend on only half the number of coordinates on M . Therefore one introduces a polarization F which is a complex distribution

on TM of dimension $n = \frac{1}{2} \dim M$ satisfying the following conditions:

- $$\left. \begin{array}{l} \text{(i) } F_m \subset (T_m M)^{\mathbb{C}}, \quad \dim_{\mathbb{C}} F_m = n \\ \text{(ii) } F \text{ is isotropic} \\ \text{(iii) } F \text{ is involutive} \\ \text{(iv) } \dim_{\mathbb{C}} F^{\dagger} \cap F = k \text{ is constant on } M \end{array} \right\} \Leftrightarrow F \text{ is lagrangian}$$

(v) $F^\dagger + F$ is involutive.

Conditions (i) to (iii) say essentially that a function which is constant on the leaves of F depends only on the first n coordinates of a canonical coordinate system; conditions (iv) and (v) are technical conditions.

The polarisation F we will use when quantizing the (reduced) hydrogen atom, is spanned by either of the following three sets of five (local) vectorfields:

$$(3.1) \quad \{\partial/\partial \mathbf{v}, \partial/\partial z_1^\dagger, \partial/\partial z_2^\dagger\}, \quad \{\partial/\partial \mathbf{p}, \partial/\partial z_1^\dagger, \partial/\partial z_2^\dagger\}$$

$$(3.2) \quad \text{or } \{\mathbf{X}_r, \mathbf{X}_{z_1}, \mathbf{X}_{z_2}\}$$

where z_i ($i = 1, 2$ indicating the first and second particle) is a (local) complex-holomorphic coordinate on $S^2 = \mathbb{P}^1(\mathbb{C})$ with respect to the complex structure introduced in §2b. Roughly speaking H_c will be replaced by a Hilbert-space H consisting of «functions» which are constant along the polarization F , which means in this case of functions of \mathbf{r} and z_i which are holomorphic in z_i .

It is from this point on that the quantization formalism of Souriau diverges from the formalism of Kostant, so the (results of the) different quantization procedures will be discussed in the next section.

§4. QUANTIZATION

The basic idea in both quantization formalisms is to compute the flow a_t associated to the hamiltonian vectorfield X_H (1.9), lift this flow to a flow \hat{a}_t on the Hilbert-space H , and finally compute $\hat{a}_t(\Psi)$ up to first order in t :

$$\hat{a}_t(\Psi) = \Psi + i/\hbar \mathbb{H} \Psi t + O(t^2)$$

where the coefficient in t is interpreted as the result of the hamiltonian-operator acting on Ψ : the generator of time evolution.

The main computational ingredient to compute this first order term is the method of stationary phase (see [Hö], lemma 7.7.3): for $\beta t \neq 0$:

$$(4.1) \quad \int_{\mathbb{R}^3} e^{3i\pi \cdot \text{sign}(\beta t)/4} (\pi t/\beta)^{-3/2} \exp(-i\beta \|\mathbf{x}\|^2/t) \mathbf{f}(\mathbf{x}) d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \\ = \mathbf{f}(\mathbf{0}) - it/4\beta [\Delta_{\mathbf{x}} \mathbf{f}](\mathbf{0}) + O(t^2).$$

Remark. In the sequel of this section we will often say that the Hilbert-space H is given by a certain vector space with an inner-product. In reality this space will only be a pre-Hilbert-space but we have adopted this language for the sake brevity. The reader is asked to interpret these statements as « H is the completion

of the inner-product space», e.g.:

$$L^2(\mathbb{R}) = \{C^\infty \text{ functions on } \mathbb{R}\}.$$

§4a. QUANTIZATION WITH POLARIZERS

In the quantization scheme of Souriau [Sol], given a polarization F of (M, σ) and a prequantization (Y, α) , one deals with the complex distribution F^\wedge of TY defined by:

$$(4.2) \quad \alpha(F^\wedge) = 0, \quad F = \pi_* F^\wedge$$

which is called a *Planck-polarization* (the horizontal lift of F). Then the Hilbert-space H of wave functions is the space of C^∞ functions $f: Y \rightarrow \mathbb{C}$ satisfying:

$$\begin{cases} F^\wedge f = 0 \\ \forall \xi \in U(1) : \xi^* f = \xi \cdot f \end{cases}$$

where on the left-hand side ξ denotes the action of $U(1)$ on the principal bundle Y and on the right-hand side ξ denotes multiplication by the complex number ξ .

In our case Y is a quotient from $T^*Q \times S^3 \times S^3$ which is in turn embedded in $T^*Q \times \mathbb{C}^2 \times \mathbb{C}^2$. Now we will always use the coordinates $(\mathbf{r}, \mathbf{v}, \mathbf{Z}_1, \mathbf{Z}_2)$ on $T^*Q \times \mathbb{C}^2 \times \mathbb{C}^2$, but it goes without saying that the expressions given will descend to Y . So the Planck-polarization F^\wedge (which is 5 dimensional) associated to the polarization (3.1) is given by the trace on Y of the mixed real/complex distribution on $T^*Q \times \mathbb{C}^2 \times \mathbb{C}^2$ spanned by the 7 vectorfields:

$$\partial/\partial \mathbf{v}, \quad \partial/\partial \mathbf{Z}_1, \quad \partial/\partial \mathbf{Z}_2$$

(N.B. beware of the relation between (Z^1, Z^2) (as defined in §2a) and z (as defined in §2b): $z^\dagger = Z^1/Z^2$, which holds for both particles). The associated Hilbert-space is given by:

$$(4.3) \quad H = \{f(\mathbf{r}, \mathbf{v}, \mathbf{Z}_1, \mathbf{Z}_2) = \sum_{\alpha, \beta=1,2} \Psi(\mathbf{r})_{\alpha\beta} Z_1^{\alpha\dagger} Z_2^{\beta\dagger}, \quad \|f\|^2 < \infty\}$$

or equivalently by:

$$(4.4) \quad H = \{\Psi(\mathbf{r})_{\alpha\beta} | \alpha, \beta = 1, 2 \text{ and } \|\Psi\|^2 < \infty\}$$

where the norm $\| \cdot \|$ is derived from the hermitian scalar product $\langle \cdot, \cdot \rangle$ defined by

$$\langle f, g \rangle = (2\pi)^{-2} \int_{Q \times S^2 \times S^2} f \cdot g^\dagger \, d\mathbf{r} \, d\mathbf{u}_1 \, d\mathbf{u}_2$$

or

$$\langle \Psi, \Phi \rangle = \sum_{\alpha, \beta=1,2} \int_{\mathbb{R}^3} \Psi(\mathbf{r})_{\alpha\beta} \Phi(\mathbf{r})_{\alpha\beta}^\dagger d\mathbf{r}.$$

It is worth noticing that the Planck polarization F^\wedge (4.2) can be viewed as the kernel of the derivative $d\phi$ of the complex 5-form ϕ on Y :

$$\phi = \text{vol}(\mathbf{Z}_1, d\mathbf{Z}_1)^\dagger \wedge \text{vol}(\mathbf{Z}_2, d\mathbf{Z}_2)^\dagger \wedge d\mathbf{r}^1 \wedge d\mathbf{r}^2 \wedge d\mathbf{r}^3$$

where $\text{vol}(\mathbf{Z}, d\mathbf{Z}) = Z^1 dZ^2 - Z^2 dZ^1$.

It can be shown that this 5-form satisfies the conditions:

$$(4.5) \quad \begin{cases} \text{(i)} & d\phi = ik/\hbar \alpha \wedge \phi \\ \text{(ii)} & \text{rank}(\phi) = n \end{cases}$$

where $k \in \mathbb{Z} \setminus \{0\}$ (here $k = 2$) and $n = \frac{1}{2} \dim(M)$ ($= 5$). Any complex n -form satisfying these conditions is called a k -polarizer and the (complex) distribution F^\wedge defined by:

$$F^\wedge = \ker(d\phi)$$

is a Planck polarization. For an introductory account, see [Du] and [Ra]. One of the subtleties with polarizers is the rising of certain global existence conditions, which leads to strong selection rules on the (prequantizable) symplectic manifolds (e.g. only spins $\frac{1}{2}$ and 1 can be «polarized» in a $SU(2)$ -invariant way; fortunately enough this is the case of our model).

Using the polarizer ϕ we can describe the Hilbert-space H (4.3) as the set of those C^∞ functions $f: Y \rightarrow \mathbb{C}$ satisfying:

$$(4.6) \quad (df - i/\hbar f \alpha) \wedge \phi = 0.$$

Let a_t denote the flow of the Hamiltonian vectorfield X_H on (M, σ) (see (1.9)) and \hat{a}_t the flow of X_H^\wedge on (Y, α) (see (2.1)). The flow \hat{a}_t is a local 1-parameter group of diffeomorphisms of (Y, α) which leaves α invariant and commutes with the action of $U(1)$. Trivially, $\phi_t = \hat{a}_t^* \phi$ is again a polarizer (i.e. satisfying conditions (4.5)) with associated Hilbert space H_t as defined by (4.6). Since $f_t = f \circ \hat{a}_t$ is in H_t if f is in H , it is possible to define a pairing between H_t and H by:

$$(4.7) \quad \langle f_t, g \rangle = \kappa \int_M f_t \cdot g^\dagger \cdot \sqrt{|\phi_t \wedge \phi^\dagger|} / \lambda \cdot \lambda$$

where λ is the Liouville volume of (M, σ) ; since $\phi_t \wedge \phi^\dagger$ is a volume form on M it is proportional to λ with proportionality function $\phi_t \wedge \phi^\dagger / \lambda$. If $\phi_t \wedge \phi^\dagger$ is nowhere zero (i.e. the polarization F transverse to the polarization $a_{t*} F$) then (4.7) defines a linear map from H_t to H and hence an evolution operator (also called \hat{a}_t) on H by:

$$(4.8) \quad \langle \hat{a}_t(f), g \rangle = \langle f_t, g \rangle.$$

If the constant κ in (4.7) can be chosen such that the expansion (4.1) holds (and in our case we can) then the flow a_t (4.8) on H defines a Hamiltonian operator \mathbf{H} .

In the case of the hydrogen atom the pairing (4.7) of polarizers reads:

$$(4.9) \quad \begin{aligned} \langle f_t, g \rangle &= (2\pi)^{-2} (2\pi m \hbar)^{-3/2} e^{3i\pi \text{sign}(\hbar)/4} \cdot \\ &\cdot \int_{T^*Q \times S^2 \times S^2} \exp(-i/\hbar \int_0^t (v \circ a_s)(\mathbf{r}, \mathbf{v}, \mathbf{Z}_1, \mathbf{Z}_2) ds) \cdot \\ &\cdot (\Sigma_{\alpha, \beta=1,2} \Psi(\mathbf{r}(t))_{\alpha\beta} Y_1^\alpha(t)^\dagger Y_2^\beta(t)^\dagger) \cdot \\ &\cdot (\Sigma_{\gamma, \delta=1,2} \Phi(\mathbf{r})_{\gamma\delta} Y_1^{\gamma\dagger} Y_2^{\delta\dagger})^\dagger \cdot \mathbf{K}_t \cdot d\mathbf{r} d(m\mathbf{v}) d\mathbf{u}_1 d\mathbf{u}_2 \end{aligned}$$

where

$$f(\mathbf{r}, \mathbf{v}, \mathbf{Z}_1, \mathbf{Z}_2) = \Psi(\mathbf{r})_{\alpha\beta} Z_1^{\alpha\dagger} Z_2^{\beta\dagger}, \quad g(\mathbf{r}, \mathbf{v}, \mathbf{Z}_1, \mathbf{Z}_2) = \Phi(\mathbf{r})_{\alpha\beta} Z_1^{\alpha\dagger} Z_2^{\beta\dagger},$$

$$Y_j(t) = Z_j(t) \cdot \exp(-i/\hbar \int_0^t (v_j \circ a_s)(\mathbf{r}, \mathbf{v}, \mathbf{Z}_1, \mathbf{Z}_2) ds) \quad (j = 1, 2) \text{ (cf. (2.1))},$$

$$(\mathbf{r}(t), \mathbf{v}(t), \mathbf{Z}_1(t), \mathbf{Z}_2(t)) = a_t(\mathbf{r}, \mathbf{v}, \mathbf{Z}_1, \mathbf{Z}_2) \quad \text{and} \quad K_t = \sqrt{|\phi_t \wedge \phi^\dagger / \lambda|}.$$

The expression given for the constant κ contains the standard normalization coefficients together with a phase factor corresponding to the Maslov index. One can show that:

$$K_t = t^{3/2} [1 + at^2 + b_j v^j t^2 + O(t^3)]$$

and

$$\begin{aligned} &\exp(-i/\hbar \int_0^t (v \circ a_s)(\mathbf{r}, \mathbf{v}, \mathbf{Z}_1, \mathbf{Z}_2) ds) \\ &= \exp(-itm \|\mathbf{v}\|^2 / 2\hbar) [1 + it/\hbar (e_1 e_2 V(\mathbf{r}) - \mu_1 \mu_2 \mathbf{u}_1 \cdot \mathbf{C}'(\mathbf{r}) \cdot \mathbf{u}_2) + \gamma t^2 + O(t^3)] \end{aligned}$$

where a, b_j ($j = 1, 2, 3$) and γ are independent of \mathbf{v} . In view of this last expression we want to apply the method of stationary phase to the integration over \mathbf{v} . Since the vectorfield X_H is linear in the velocity \mathbf{v} , the flows a_t and \hat{a}_t are analytic in \mathbf{v} and hence we can apply the method of stationary phase to each term separately in the expansion of the integrand of (4.9) with respect to \mathbf{v} . It follows (because we also have analyticity in t) that only the coefficients of $\|\mathbf{v}\|^0 t$ and $\|\mathbf{v}\|^2 t^2$ will contribute nontrivially to the 1st order in t (the Hamiltonian). Integration on spheres is achieved by using some classical formulas on the integral over S^2 of the trace of polynomials of \mathbb{R}^3 and we finally get the result:

$$\begin{aligned} (\mathbf{H}\Psi)_{\alpha\beta} = & -\hbar^2/2m \Delta_{\mathbf{r}} \Psi_{\alpha\beta} + e_1 e_2 V(\mathbf{r}) \Psi_{\alpha\beta} \\ & - \lambda_1/m \boldsymbol{\sigma}_\alpha^\gamma \cdot (\mathbf{C}(\mathbf{r}) \times \hbar/i \nabla_{\mathbf{r}} \Psi_{\gamma\beta}) - \lambda_2/m \boldsymbol{\sigma}_\beta^\gamma \cdot (\mathbf{C}(\mathbf{r}) \times \hbar/i \nabla_{\mathbf{r}} \Psi_{\alpha\gamma}) \\ & + 5/9 \mu_1 \mu_2 \Sigma_{j,k} (\sigma^j)_\alpha^\gamma \cdot \mathbf{C}'(\mathbf{r})^{jk} \cdot (\sigma^k)_\beta^\delta \cdot \Psi_{\gamma\delta} \\ & + (\lambda_1^2 + \lambda_2^2)/m \|\mathbf{C}(\mathbf{r})\|^2 \Psi_{\alpha\beta} + \lambda_1 \lambda_2/m \Sigma_{j,k} (\sigma^j)_\alpha^\gamma \cdot D(\mathbf{r})^{jk} \cdot (\sigma^k)_\beta^\delta \cdot \Psi_{\gamma\delta} \end{aligned}$$

with $D(\mathbf{r})^{jk} \equiv \delta^{jk} \|\mathbf{r}\|^{-4} - r^j r^k \|\mathbf{r}\|^{-6}$.

If we omit the wave functions, denote by $\boldsymbol{\sigma}_j$ the Pauli-matrices acting on the j -th index of the wave function ($j = 1, 2$) and introduce $\boldsymbol{\sigma}^\# = \lambda_1 \boldsymbol{\sigma}_1 + \lambda_2 \boldsymbol{\sigma}_2$ (cf. (1.2)) then we obtain the Hamiltonian operator \mathbf{H} as expressed with respect to the representation (4.4) of the Hilbert-space H :

$$\begin{aligned} (4.10) \quad \mathbf{H} = & -\hbar^2/2m \Delta_{\mathbf{r}} + e_1 e_2 V(\mathbf{r}) \\ & - \boldsymbol{\sigma}^\# \cdot (\mathbf{C}(\mathbf{r}) \times \hbar/i \nabla_{\mathbf{r}})/m + 5/9 \mu_1 \mu_2 \boldsymbol{\sigma}_1 \cdot \mathbf{C}'(\mathbf{r}) \cdot \boldsymbol{\sigma}_2 \\ & + (\lambda_1^2 + \lambda_2^2)/m \|\mathbf{C}(\mathbf{r})\|^2 + \lambda_1 \lambda_2/m (\boldsymbol{\sigma}_1 \times \mathbf{C}(\mathbf{r})) \cdot (\boldsymbol{\sigma}_2 \times \mathbf{C}(\mathbf{r})). \end{aligned}$$

§ 4b. QUANTIZATION WITH $\left(-\frac{1}{2}\right)$ -F-FORMS

Since it is outside the scope of this paper to give a complete description of this quantization method, we only give the necessary intermediate results together with some remarks for those readers who know about this method.

Using the polarization defined by either (3.1) or (3.2) we obtain a Hilbert-space H which can be represented by functions of \mathbf{r}, z_1 and z_2 ($\mathbf{r} \in \mathbb{R}^3, z_i \in \mathbb{C}$) which are polynomials of degree $(2s_i/\hbar - 1)$ in z_i . If we specialise to the case $s_1 = s_2 = \hbar$ we obtain spin-spaces of dimension 2 for each spin, corresponding to particles with spin $\frac{1}{2}$. It should be noted that the use of $\left(-\frac{1}{2}\right)$ -F-forms gives us a spin-shift of one half with respect to the previous method (which is

equivalent to using $\left(-\frac{1}{2}\right)$ - F -densities; see §4c) (see also [Wo], §6.3.6 and [Tu2]); the reader is referred to the discussion in §5 for more comments on this difference. In our case the Hilbert-space can now be given as:

$$(4.11) \quad H = \{ \psi(\mathbf{r}, z_1, z_2) = \sum_{\alpha, \beta=0,1} \Psi(\mathbf{r})_{\alpha\beta} z_1^\alpha z_2^\beta (z_1 z_1^\dagger + 1)^{-1} (z_2 z_2^\dagger + 1)^{-1} \mid \\ \Psi \text{ is «square integrable»} \}$$

with inner-product

$$(4.12) \quad \langle \psi, \varphi \rangle = 16\hbar^2 \int_{\mathbb{R}^3 \times \mathbb{C}^2} d\mathbf{r} dx_1 dy_1 dx_2 dy_2 (z_1 z_1^\dagger + 1)^{-2} (z_2 z_2^\dagger + 1)^{-2} \cdot \\ \cdot \sqrt{\det A} \psi(\mathbf{r}, z_1, z_2)^\dagger \varphi(\mathbf{r}, z_1, z_2) \\ \text{with } \sqrt{\det A} = (2\hbar\hbar)^{-1} (z_1 z_1^\dagger + 1) (z_2 z_2^\dagger + 1)$$

or equivalently by

$$(4.13) \quad H = \{ \Psi(\mathbf{r})_{\alpha\beta} \mid \text{square-integrable, } \alpha, \beta = 0, 1 \}$$

with inner-product

$$\langle \Psi, \Phi \rangle = \pi \cdot \sum_{\alpha, \beta=0,1} \int_{\mathbb{R}^3} \Psi(\mathbf{r})_{\alpha\beta}^\dagger \Phi(\mathbf{r})_{\alpha\beta} d\mathbf{r}.$$

Remarks.

1) In the cases Z_j^α , r^k and σ^k the superscripts α and k denote the α -th and k -th component of the vectors Z_j , \mathbf{r} and $\boldsymbol{\sigma}$; however the superscript α in z_j^α denotes an exponent.

2) ψ and φ can be seen as the local (i.e. on the chart U_{++}) expressions of sections of the prequantum bundle L , sections which are covariant constant along the polarisation F .

3) The $\left(-\frac{1}{2}\right)$ - F -forms are chosen such that they are identically 1 on the meta-frame corresponding to the frames of F given in (3.2).

4) The first line in (4.12) is derived from the Liouville measure associated to the symplectic form σ given in (1.8) by substituting the three vectorfields $-\partial/\partial \mathbf{p} \equiv X_r$. On S^2 we use the local complex coordinate $z = x + iy$ as defined in §2b, in which the surface is given by

$$\text{surf.} = 4(x^2 + y^2 + 1)^{-2} dy \wedge dx.$$

5) $\sqrt{\det A}$ is a correcting factor to insure that the expression is a correct density on $\mathbb{R}^3 \times \mathbb{C}^2$.

6) The second, more convenient formulation of H can be computed directly from the first one by integrating over \mathbb{C}^2 .

If a_t is the flow associated to the hamiltonian vectorfield X_H (1.9) then the flow \hat{a}_t on H is defined by the BKS (Blattner-Kostant-Sternberg)-kernel:

$$(4.14) \quad \langle \psi, \hat{a}_t(\varphi) \rangle = 16\hbar^2 \int_{\mathbb{R}^6 \times \mathbb{C}^2} d\mathbf{r} d\mathbf{p} dx_1 dy_1 dx_2 dy_2 (z_1 z_1^\dagger + 1)^{-2} (z_2 z_2^\dagger + 1)^{-2} \cdot \\ \cdot \sqrt{\det A_t} \psi(\mathbf{r}, z_1, z_2)^\dagger (\varphi \circ a_t)(\mathbf{r}, \mathbf{p}, z_1, z_2) \cdot \\ \cdot \exp(i\hbar)^{-1} \int_0^t (\vartheta(X_H) - H)(a_s(\mathbf{r}, \mathbf{p}, z_1, z_2)) ds$$

with A_t a 5×5 matrix given by:

$$A_t = \begin{pmatrix} (i\hbar)^{-1} X_{r^k}(r^l \circ a_t) & (i\hbar)^{-1} X_{r^k}(z_\lambda \circ a_t) \\ (i\hbar)^{-1} X_{z_\kappa}(r^l \circ a_t) & (i\hbar)^{-1} X_{z_\kappa}(z_\lambda \circ a_t) \end{pmatrix}.$$

Remarks

- 1) Here the first part is the complete Liouville measure.
- 2) $(\varphi \circ a_t) \cdot \exp(\dots \int \dots ds)$ is the local expression of the time-evolution of the section φ of the prequantization line bundle L .
- 3) $\sqrt{\det A_t}$ is again a correcting factor to insure that the integral is a well defined density on $\mathbb{R}^6 \times \mathbb{C}^2$.
- 4) Since $a_{t*}F$ and F^\dagger are transversal for small t , no extra terms representing the $\left(-\frac{1}{2}\right)$ -forms are involved.

Finally we compute the term linear in t in the integral (4.14), using the flow (1.9) and the method of stationary phase (4.1). When we evaluate the integrals over \mathbb{C}^2 , using the second representation of the Hilbert-space, the result is given by the hamiltonian:

$$(4.15) \quad \mathbb{H} = -\hbar^2/2m \Delta_r + e_1 e_2 V(\mathbf{r}) \\ - \boldsymbol{\sigma}^\# \cdot (\mathbf{C}(\mathbf{r}) \times \hbar/i \nabla_r)/2m + 2/9 \mu_1 \mu_2 \boldsymbol{\sigma}_1 \cdot \mathbf{C}'(\mathbf{r}) \cdot \boldsymbol{\sigma}_2 \\ + (\lambda_1^2 + \lambda_2^2)/4m \|\mathbf{C}(\mathbf{r})\|^2 + \lambda_1 \lambda_2/4m (\boldsymbol{\sigma}_1 \times \mathbf{C}(\mathbf{r})) \cdot (\boldsymbol{\sigma}_2 \times \mathbf{C}(\mathbf{r}))$$

where $\boldsymbol{\sigma}^\# = \lambda_1 \boldsymbol{\sigma}_1 + \lambda_2 \boldsymbol{\sigma}_2$ (compare with (1.2)) and where the matrices $\boldsymbol{\sigma}_j$ act

upon the j -th index of $\Psi_{\alpha\beta}$, i.e. σ_1 act upon index α and σ_2 upon β .

§4c. QUANTIZATION WITH $\left(-\frac{1}{2}\right)$ -F-DENSITIES

When using $\left(-\frac{1}{2}\right)$ -F-densities instead of $\left(-\frac{1}{2}\right)$ -F-forms there is apparently no change in the Hilbert-space: it is, apart from an overall factor, given by (4.11) (or equivalently by (4.13)). The most important difference is that one has to use $s_1 = s_2 = \frac{1}{2} \hbar$ instead of $s_1 = s_2 = \hbar$ to derive this result. This difference can be attributed to the fact that the $\left(-\frac{1}{2}\right)$ -F-form which is 1 on the metaframe corresponding to the frame (3.2) is a $\left(-\frac{1}{2}\right)$ -F-form which is covariant constant along F , while the $\left(-\frac{1}{2}\right)$ -F-density which is 1 on the frame (3.2) is not. On the other hand the $\left(-\frac{1}{2}\right)$ -F-density which takes the value $(z_1 z_1^\dagger + 1)^{-\frac{1}{2}} (z_2 z_2^\dagger + 1)^{-\frac{1}{2}}$ on the frame (3.2) is a covariant constant $\left(-\frac{1}{2}\right)$ -F-density. Another difference is that $\sqrt{\det A}$ should be replaced by $\sqrt{|\det A|}$, but since $\det A$ is real positive, this change is not visible.

The difference between forms and densities becomes visible when we calculate $\langle \psi, a_t(\varphi) \rangle$ with the BKS-kernel for $\left(-\frac{1}{2}\right)$ -F-densities: $\sqrt{\det A_t}$ has to be replaced by $\sqrt{|\det A_t|}$ times a factor of modulus 1: the Maslov index (see also §4a). Moreover the calculations of a_t has to be done with $s_1 = s_2 = \frac{1}{2} \hbar$ instead of $s_1 = s_2 = \hbar$. Apart from those changes, the same remarks as for the BKS-kernel with forms are valid. In this case one obtains the hamiltonian \mathbb{H} :

$$(4.16) \quad \begin{aligned} \mathbb{H} = & -\hbar^2/2m \Delta_r + e_1 e_2 V(r) \\ & - \sigma^\# \cdot (C(r) \times \hbar/i \nabla_r)/m + 5/9 \mu_1 \mu_2 \sigma_1 \cdot C'(r) \cdot \sigma_2 \\ & + (\lambda_1^2 + \lambda_2^2)/m \|C(r)\|^2 + \lambda_1 \lambda_2/m (\sigma_1 \times C(r)) \cdot (\sigma_2 \times C(r)) \end{aligned}$$

which is exactly equal to the result (4.10) obtained by quantization with polarizers.

§5. DISCUSSION

The results of the two quantization methods (which we will call the polarizer

method and the $\frac{1}{2}$ -form method) are given in (4.10) and (4.15). The fact that these two methods give different results (although only in some numerical constants) should not be surprising since they quantize different symplectic manifolds (polarizers $s_1 = s_2 = \frac{1}{2} \hbar \leftrightarrow \left(-\frac{1}{2}\right)$ - F -forms $s_1 = s_2 = \hbar$). The justification of these different models is given by the interpretation of the parameter s (or equivalently by the resulting quantum Hilbert-space); however, the authors could not decide which procedure is the right one, since both methods do not really arrive at the correct answer.

Before we discuss the different terms in more detail, we make two global comments. First we note that we have omitted the origin of \mathbb{R}^3 from our configuration space because of the singularity at $\mathbf{r} = \mathbf{0}$ of the Coulomb potential. However we have reintroduced the origin in the description of our Hilbert-space, which consists of four copies of $L^2(\mathbb{R}^3, \text{Lebesgue})$. This manipulation is completely justified by the isomorphism $L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3 \setminus \{\mathbf{0}\})$ (given by restriction of functions) between Hilbert-spaces. The second remark concerns the interpretation of the model: the reduced model as given in §1 does **not** describe the motion of the electron, although it does to a fairly good approximation since the reduced mass is nearly equal to the electron mass (an «infinitely heavy» proton). Consequently our model incorporates from the beginning the correction that one has to use the reduced mass instead of the electron mass.

We now consider the different terms in (4.10) and (4.15) separately while substituting the correct values for the charges, magnetic moments and masses, interpreting the first particle as the electron and the second particle as the proton; more precisely:

$$\begin{array}{ll}
 m_1 = m_e & m_2 = m_p \quad m = \text{reduced mass} = m_1 m_2 / (m_1 + m_2) \approx m_e \\
 e_1 = -e & e_2 = e \quad e = \text{elementary (positive) charge} \\
 \mu_1 = -g_e e \hbar / (4 m_e c) & \mu_2 = g_p e \hbar / (4 m_p c) \\
 \lambda_1 = -g_e e^2 \hbar / (4 m_e c^2) & \lambda_2 = -g_p e^2 \hbar / (4 m_p c^2) \\
 g_e = \text{electron } g\text{-value} \approx 2.0 & g_p = \text{proton } g\text{-value} \approx 5.6.
 \end{array}$$

To facilitate the comparison with literature (e.g. [B&S], [Co] or [Ga]) we also introduce the operators angular momentum \mathbf{L} , electron-spin \mathbf{S} and proton-spin \mathbf{I} defined as:

$$\mathbf{L} = \mathbf{r} \times \hbar/i \nabla_{\mathbf{r}} \quad \mathbf{S} = \frac{1}{2} \hbar \boldsymbol{\sigma}_1 \quad \mathbf{I} = \frac{1}{2} \hbar \boldsymbol{\sigma}_2.$$

With these conventions we obtain the following terms.

1) *Kinetic energy and Coulomb potential*

$$-\frac{\hbar^2}{2m} \Delta_{\mathbf{r}} - \frac{e^2}{\|\mathbf{r}\|}.$$

These terms are well known and need no comment.

2) *Electron spin-orbit coupling*

$$\left(1 \text{ or } \frac{1}{2}\right) \cdot \frac{g_e e^2}{2m_e c^2} \cdot \frac{1}{\|\mathbf{r}\|^3} \cdot \mathbf{S} \cdot \mathbf{L}.$$

Here we note for the first time a difference: the polarizer method obtains a factor 1, the $\frac{1}{2}$ -form method finds a factor $\frac{1}{2}$ and in literature one finds a factor $\frac{1}{2}$ with a footnote saying that a heuristic reasoning gives a factor 1 but due to Thomas precession the correct value should be $\frac{1}{2}$. It seems that the $\frac{1}{2}$ -form method obtains the correct factor; on the other hand, the purely phenomenological constant k (introduced in (1.2)) was given the value $k = c^{-1}$ by Souriau to be compatible with the macroscopic theory of magnetism. Hence nothing hinders us to make another choice, e.g. $k = \frac{1}{2} c^{-1}$, to obtain the correct factor in the spin-orbit coupling when using the polarizer method (showing that the correct value obtained by the $\frac{1}{2}$ -form method is accidental).

3) *Spin-spin interaction*

$$(5/9 \text{ or } 2/9) \cdot \frac{g_e g_p e^2}{4m_e m_p c^2} \cdot \left[-\frac{\mathbf{S} \cdot \mathbf{I}}{\|\mathbf{r}\|^3} + 3 \frac{(\mathbf{S} \cdot \mathbf{r})(\mathbf{I} \cdot \mathbf{r})}{\|\mathbf{r}\|^5} \right].$$

Again different constants: 5/9 by the polarizer method, 2/9 by the $\frac{1}{2}$ -form method and 1 in literature! Before we discuss the different constants we note that the operator in square brackets contains a singularity in the origin; in the usual way (see [Ga] or [B&S]) one deduces that this singularity has the form of a delta function $\delta(\mathbf{r})$. This delta function contribution is sometimes called the Fermi-contact term and it explains the hyperfine structure of the spectrum of the hydrogen atom (the 21.4 cm radio wave in astronomy) which is verified experimentally to a very high degree of accuracy. It shows that the constants

obtained by both methods are incorrect. Moreover, the $\frac{1}{2}$ -form method, which was originally introduced to obtain the correct energy spectrum of the harmonic oscillator (metaplectic correction), does not in this case correct the spectrum correctly.

It is our opinion that this is a serious problem which seems to be intimately related to the use of complex polarizations. One might hope that systematic use of real polarizations (even if they have singularities, which is unavoidable on S^2) leads to the correct answer. Research is being done in this direction.

4) Proton spin-orbit interaction

$$\left(1 \text{ or } \frac{1}{2}\right) \cdot \frac{g_p e^2}{2m_p c^2} \cdot \frac{1}{\|\mathbf{r}\|^3} \cdot \mathbf{I} \cdot \mathbf{L}.$$

This term has the same form as the electron spin-orbit interaction but is negligible with respect to it since the ratio $m_p/m_e \approx 2000$. Apart from this consideration, the same remarks as given for the electron spin-orbit interaction apply in this case.

5) Diamagnetic terms

$$\left(1 \text{ or } \frac{1}{4}\right) \cdot \left[\frac{\lambda_1^2 + \lambda_2^2}{m \|\mathbf{r}\|^4} + \frac{\lambda_1 \lambda_2}{m \|\mathbf{r}\|^6} \cdot (\boldsymbol{\sigma}_1 \times \mathbf{r}) \cdot (\boldsymbol{\sigma}_2 \times \mathbf{r}) \right].$$

These terms are of the order c^{-4} (they contain λ^2) and hence negligible with respect to the terms 1), 2) and 3) which are of the order 1 or c^{-2} . The origin of the difference in constants here is the same as in the second term but appears here squared because it is quadratic in the parameters λ .

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